Table I. Column 4, labelled f, lists isotopic abundance fractions from Anders and Grevesse [11]. Columns 5 through 7 are from Table of Isotopes [12]. Column 5, labelled I, is the nuclear spin. Column 6, labelled μ, is the magnetic dipole moment in nuclear magnetons. Column 7, labelled Q, is the electric quadrupole moment in barns. Q is identically 0 for spin 1/2.

Fig. 1. A small section of the solar central intensity spectrum at 692.5 nm plotted at full scale and at 10 times scale. The heavy lines show the observed FTS spectrum from James Brault at Kitt Peak. The resolution is 522000 and the signal-to-noise is about 3000 which is poor for this work. The continuum level is uncertain. The thin line is the computed spectrum. It would be possible to adjust the line data for a better match but most of the discrepencies are from missing lines. There are solar lines of Ca I, Ti I, Cr I, Fe I, C I, CN, and terrestrial lines of H_2O and $^{16}O^{18}O$. The first number in each line label is the last 3 digits of the wavelength and the 4th number is the per mil central intensity if the line were computed in isolation.

Fig. 2. A small section of the solar central intensity spectrum at 599 nm plotted at full scale and at 10 times scale. The heavy lines show the observed FTS spectrum from James Brault at Kitt Peak. The resolution is 522000 and the signal-to-noise is about 3500 which is poor for this work. The continuum level is very uncertain due to atmospheric ozone. The thin lines are the computed spectrum. There are solar lines of Ca I, Ti I, Cr I, Cr II, Fe I, Fe II, Co I, Yb II, C_2, and terrestrial lines of H_2O. The first number in each line label is the last 3 digits of the wavelength and the 4th number is the per mil central intensity if the line were computed in isolation. The Co I line at 599.1866 has been divided into 15 hyperfine components. The hyperfine splitting is not known for the two other Co I lines. There are many missing lines.

Fig. 3. Resolved isotopic splitting profiles for Fe II and Ni II redrawn after [13]. The indications for ^{61}Ni and ^{57}Fe, which are hyperfine split, were added because of excess emission at those wavelengths.

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Table I. Stable isotopes

Z	A	f	I	μ	Q	Z	A	f	I	μ	Q	Z	A	f	I	μ

including all the predicted lines. Unfortunately, this will produce 10 times as many lines.

Acknowledgements

This work is supported in part by NASA grants NSG-7054, NAG5-824, and NAGW-1486. The most important contribution to this work is a large grant of Cray computer time at the San Diego Supercomputer Center.

References

1. Kurucz, R. L. and Furenlid, I., Smithsonian Astrophys. Observ. Spec. Rep. No. 387, (1981).
2. Kurucz, R.L. and Avrett, E.H., Smithsonian Astrophys. Observ. Spec. Rep. No. 391, (1981).
3. Vernazza, J. E., Avrett, E. H., and Loeser, R., Ap. J. Suppl. **45**, 635 (1981).
4. Kurucz, R.L., Smithsonian Astrophys. Observ. Spec. Rep. No. 309, (1970).
5. Peterson, D. M., Personal communication (1979).
6. Vidal, C.R., Cooper, J., and Smith, E.W., Ap. J. Suppl. **25**, 37 (1973).
7. Rothman, L. S., Gamache, R. R., Goldman, A., Brown, L. R., Toth, R. A., Pickett, H. M., Poynter, R. L., Flaud, J.-M., Camry-Peyret, C., Barbe, A., Husson, N.,Rinsland, C. P., and Smith, M. A. H., Appl. Optics **26**, 4058 (1987).
8. Kurucz, R. L., Rev. Mexicana Astron. Astrof. **23**, 45 (1992).
9. Kurucz, R. L., Rev. Mexicana Astron. Astrof. **23**, 187 (1992).
10. Brault, J.W. and Holweger, H., Ap. J. Lett **249**, L43 (1981).
11. Anders, E. and Grevesse, N., Geochimica et Cosmochimica Acta **53**, 197 (1989).
12. Lederer, C. M. and Shirley, V. S., eds., "Table of Isotopes", Wiley, New York (1978).
13. Kurucz, R. L., submitted to Ap. J. Lett. (1992).
14. Rosberg, M., Litzén, U., and Johansson, S., this volume (1992).
15. Hühnermann, H., this volume (1992).
16. Booth, A. J. and Blackwell, D. E., Mon. Not. R. Astr. Soc., **204**, 777 (1983).
17. Cowley, C. R. and Frey, M., Ap. J. **346**, 1030 (1989).
18. Hühnermann, H., personal communication (1992).

Table I Caption. Column 4, labelled f, lists isotopic abundance fractions from Anders and Grevesse [11]. Columns 5 through 7 are from Table of Isotopes [12]. Column 5, labelled I, is the nuclear spin. Column 6, labelled μ, is the magnetic dipole moment in nuclear magnetons. Column 7, labelled Q, is the electric quadrupole moment in barns. Q is identically 0 for spin 1/2.

able to find in the literature. Only 2 lines have been measured for Ti I, 4 for Cr I, 2 for Fe I, and 44 for Ni I. No measurements have been published for ions of these elements. However if you go into James Brault's office at Kitt Peak and look through the files of infrared FTS spectra, isotopic splittings are clearly visible in the even elements and hyperfine splittings are clearly visible in the odd elements. Analysis of Brault's spectra and new laboratory measurements are urgently needed. Figure 3 is based on paper presented at this meeting by Rosberg, Litzén, and Johansson [14] in which they show the first isotopic splitting data for Fe II and Ni II. As both hyperfine splitting and the isotope shift vary roughly as Z^3 [15], higher ions will have much larger splittings.

In natural mixtures essentially all atomic lines are asymmetric because of isotopic and hyperfine components. In astrophysics the effects of these components have been generally ignored in the case of Ti, Cr, Fe, and Ni which together account for the majority of atomic lines. The effects of ignoring isotopic structure are similar to those produced by ignoring hyperfine splitting as discussed by Booth and Blackwell [16] and by Cowley and Frey [17]. Ignoring isotopic or hyperfine splitting introduces the following systematic errors: 1) the use of bisectors to determine velocity fields is incorrect; 2) Fourier analysis of line profiles to determine rotational, microturbulent, and macroturbulent velocities is incorrect; and 3) damping constants are overestimated. When the stronger components become saturated, the weak components are still on the linear part of the curve of growth. They make a larger contribution to the total feature than their fractional abundance might suggest. This introduces the additional systematic errors: 4) wavelengths of saturated lines are shifted relative to the isotopic abundance weighted position; and 5) abundances determined from equivalent widths are systematically too large. A sample curve of growth is given in [13]. Abundances should be determined by spectrum synthesis. In addition, 6) the Doppler width and Voigt profile differ significantly from isotope to isotope. Systematic errors for interstellar lines can be more pronounced than for stellar lines because their Doppler widths can be quite small.

It is imperative that laboratory measurements be made to determine the isotopic splitting of every energy level of every stable isotope of every atom and ion as is now routinely done for actinides and for diatomic molecules. The hyperfine splitting should be measured as well for those isotopes with nuclear spin. The data should be presented in a form that is directly usable. Energy level publications should list the energy levels for each isotope and for each hyperfine component when they exist.

These laboratory analyses should be performed with pure isotopes. Pure isotope hollow cathodes run at varying pressures would allow removing pressure shifts for very accurate level determination. Without the complication of multiple isotopes, lines are less blended and the spectra are easier to reduce. In general, liquid-nitrogen-cooled hollow cathodes should be used for spectrum analysis to maximize resolution. Such cathodes are used routinely in the hyperfine community because of their narrow Doppler widths [18]. While the capability still exists, Russia, the United States, and other countries should stockpile 100g samples of every stable isotope (Table I) for use in this work.

At the present time I am including hyperfine and isotopic splitting in my spectrum calculations, one level at a time, from whatever laboratory data I can find. Given enough laboratory data, it should be possible to work semiempiricially to generate the splittings for whole computed transition arrays,

very reliable. If laboratory measurements exist for such lines, the laboratory measurements are always preferable to the calculation. I collect all published data on gf values and include them in the line list whenever they appear to be more reliable than the current data.

I hope to spend the next year improving the line data. I will extend the atomic calculation to elements lighter and heavier than the iron group which I have already computed. Several of the iron group calculations have already been revised. I will recompute the energy levels and line lists whenever new laboratory analyses become available and I will make the predictions available to laboratory spectroscopists. Because computers are now more powerful, I will increase the number of configurations treated. This should account for more of the missing infrared lines because they are usually transitions between highly excited levels.

I plan to distribute tapes and CD-ROMs with files of energy levels, damping constants, Landé g values, lifetimes, branching ratios, and line gf values. These should be useful to both laboratory and astronomical spectroscopists.

5. Isotopic and Hyperfine Splitting

I am reducing solar central intensity spectra taken by James Brault with the FTS on the McMath telescope at Kitt Peak. The spectra were observed with resolving power greater than 522000 in the visible and signal-to-noise greater than 3000. I typically plot the observed and computed spectra at a wavelength scale of 2 m/nm and a residual intensity scale of 2 m. Wavelengths can be read by eye to 0.0001 nm. All lines in the spectra are blended. When the observed spectra are compared with computed spectra [9], they do not look "right": the damping wings do not look like Voigt profiles and the lines seem to be asymmetric. Because of blending and missing lines and uncertainties in continuum placement, however, this is difficult to demonstrate from the comparison. Also there are Doppler shifts and asymmetries from mass motions in the solar atmosphere on the order of 100 m/s, and many of the lines are naturally asymmetric due to hyperfine splitting. I have included hyperfine splitting in my spectrum calculations for Sc, V, Mn, and Co for lines that have laboratory data available. Removing those lines from consideration, the remaining lines still give the same impression. I wondered whether there might not be other isotopes of Ti, Cr, Fe, and Ni with hyperfine splitting that could cause an asymmetry. There are, but the effect is small. That led me to discover that there is significant isotopic splitting in these elements that has not been considered. The one exception is a paper by Brault and Holweger [10] on the isotopic splitting of Ni in the infrared. In Table I are listed all the stable isotopes of all the elements, their isotopic abundances from Anders and Grevesse [11], and the nuclear spin, the nuclear magnetic moment, and the nuclear electric quadrupole moment from the Table of Isotopes [12]. The isotopes with nuclear spin have hyperfine splitting and almost every element has at least one isotope with hyperfine splitting. The magnitudes of the magnetic moment and the spin give an indication of the strength of the hyperfine splitting. The only element that does not have isotopic or hyperfine splitting is thorium.

In [13] I show schematic isotopic splitting patterns for Ti, Cr, Fe and Ni and I list all the isotopic splitting data for Ti, Cr, Fe, and Ni that I have been

up through Zn and the first 5 ions of heavier elements up through Es. The elemental abundances are treated as variables with depth. It can treat any number of depths.

At present ATLAS12 has 6 input files containing 58,000,000 lines. For each line the wavelength, identification, lower energy level, gf value, and the radiative, Stark, and van der Waals damping constants are packed into 16 bytes. At each wavelength point in a frequency integration the Voigt profiles of all the significant nearby lines are computed and summed. Hydrogen lines, autoionizing lines, etc. can be treated with more complicated profile functions. The program and line files will be distributed in the spring of 1993.

4. Atomic and Molecular Data

Use of the programs described above depends on having reliable gf values and damping constants for atomic and molecular lines, photoionization cross-sections, and, for non-LTE problems, collision cross-sections. My work on atomic and molecular line data and my line lists are described in [8]. Here I will concentrate on the present problems and on my future work.

Accurate energy levels, accurate wavelengths, accurate gf values, and accurate damping constants are required for computing spectra. Hyperfine and isotopic splitting are also required, and for magnetic structures, Landé g values are needed. We require completeness because we need to deconvolve blends. We need every level below the lowest ionization or dissociation energy. For molecules, every vibrational and rotational level is needed, not just the ones populated at low temperatures in the laboratory.

The procedure I use for generating line lists is straightforward and produces all the lines up to a specified cut-off lower energy level. I start with all the known energy levels. I set up a model Hamiltonian that uses a Slater integral expansion for atoms or a rotational expansion for molecules. Then I do a least squares fit to determine the Slater integrals or the rotational constants. For atoms I use scaled Hartree-Fock starting guesses for the integrals. Once the fit has converged, I use the Hamiltonian to generate all possible eigenvalues and eigenvectors. The eigenvalues are replaced by the observed energies where they are known. For atoms I generate a scaled-Thomas-Fermi-Dirac wavefunction for each configuration and compute all the transition integrals. For molecules I compute the RKR potential and then all the vibrational wavefunctions. I then integrate over measured or computed transition moments taken from the literature to get the transition integrals. The transition integrals are divided into transition arrays in the adopted basis and are transformed to observed coupling using the eigenvectors. Given enough computer time, I can readily generate thousands of energy levels and millions of lines. Thus far I have produced atomic and molecular line lists with 58 million lines. Since the known energy levels are used when available, the line wavelengths are correct for lines between known energy levels. Lines to predicted levels are as accurate as the least squares fitting procedure. Radiative, Stark, and van der Waals damping constants and Landé g values are automatically produced for each line.

Problems arise when not all the "known" energy levels are really known. There are misassignments, typos, and other mistakes. Also, the Hamiltonians are approximate, so any lines that occur only because of mixing may not be

functions, in the Saha and Boltzmann equations, and in the opacities. Departure coefficients for levels that are higher than have been computed are assumed to be the same as those for the ground state of the next higher stage of ionization. If the model atmosphere is in LTE the departure coefficients are all set to unity. The program computes the non-LTE opacity and source function, adds in the LTE opacity and source function, adds the continuum opacity and source functions, and then computes the intensity or flux at each wavelength point and for each line center. Photoionization continua are put in at their exact positions, each with its own cross-section and with the series of lines that merge into each continuum included so that there are no discontinuities in the spectrum.

Hydrogen line profiles are computed using a routine from Peterson [5] that approximates the Vidal, Cooper, and Smith [6] profiles, works to high n, and includes Doppler broadening, resonance broadening, van der Waals broadening, and fine-structure splitting. Autoionization lines have Shore-parameter Fano profiles. Other lines have Voigt profiles that are computed accurately for any amount of damping. A few strong lines can be treated with approximate partial redistribution effects but the computer cost increases dramatically.

To compute a rotationally broadened flux spectrum I first compute intensity spectra at 17 angles (radial positions on the disk) and then pass them through the rotation program. A grid of, say, 10000 points is defined on the disk and, for the given projected rotation velocity $v \sin i$, the Doppler shift and angle are computed for each point. The intensity spectra are Doppler shifted and interpolated and summed over the disk to obtain the flux. In the rigid-body spherical approximation, symmetries are used to reduce the number of calculations, but the method works in the case of differential rotation as well.

To compute macroturbulent or instrumental broadening the broadening function is defined at integral values of the point spacing. Then the spectrum is read in, one wavelength at a time, redistributed among neighboring wavelengths, and added to a buffer for the new spectrum.

I also have a series of programs for computing the transmission of the spectrum through the Earth's atmosphere using the HITRAN database [7] for the line data.

The most important step in the spectrum synthesis work is the final preparation of plots because I can display enough information to study the spectrum as a whole, to compare with one or more observed spectra, to study individual features in detail, and to identify lines and the composition of blends. Figure 1 shows a small section of spectrum selected because it does not show dramatic discrepencies between the calculated and observed spectra. The figure shows raw calculations, without adjustment. Usually the fits are much worse, with many missing lines. Figure 2 shows a region that includes a Co I line for which hyperfine data are available so that all 15 components could be included.

3. New Model Atmosphere Program

I have developed a new version of my model atmosphere program, called ATLAS12, that uses opacity sampling and reads from from my whole line list. It essentially combines my spectrum synthesis program SYNTHE, described above, with my model atmosphere program ATLAS [4]. It recognizes more than 1000 species, each in up to 10 isotopic forms, including all ions of the elements

The sun is the brightest star available to us. It is possible to observe the solar spectrum with a signal-to-noise ratio of 10^4 and a resolving power of 10^6. But nobody has. In the sun we can study contributions to blends at the 1 per mil level. There are many cases where lines can be seen in the sun that have been difficult or impossible to see in the laboratory. The sun is a unique spectroscopic source for studying atoms and molecules.

I have developed computer programs for producing model stellar atmospheres and for synthesizing spectra. I am collecting and computing data on all relevant atomic and molecular lines. I check the line gf values and damping constants by comparing the computed spectra to the observed spectra. Once I can compute realistic spectra for the sun and the brightest stars these programs and data can be used to predict the spectra of stars that are too faint to observe well (or even stars from the early universe that no longer exist). Below I discuss these computer programs and the line data. Then I show how the observations and the programs have brought us to the point of requiring isotopic and hyperfine splitting data for every line.

2. Spectrum Synthesis Programs

The spectrum synthesis computer programs have been under development since 1965 and have been described by Kurucz and Furenlid [1] and by Kurucz and Avrett [2]. The algorithms for computing the total line opacity are extremely fast because maximum use is made of temperature and wavelength factorization and pretabulation. On a Cray computer a 500,000 point spectrum can be computed in one run. The same programs run on a VAX, only much more slowly. There is no limit to the number of spectrum lines that can be treated in LTE. I currently have 58,000,000. At present I can treat 50,000 lines including non-LTE effects. The line data are described below.

The spectrum calculations require a pre-existing model atmosphere that can be empirical, such as the Vernazza, Avrett, and Loeser [3] solar models, or theoretical, such as the ones I describe below. The "model atmosphere" does not have to be stellar. It can be a disk, a planetary atmosphere, a laboratory source, etc. Quantities that need be computed only once for the model atmosphere are pretabulated. There can be a depth-dependent microturbulent velocity or a depth-dependent Doppler shift.

Line data are divided into two groups for treatment. In the first group, the lines must have a source function that is either the Planck function or some function that approximately accounts for non-LTE effects in the outer layers. The first group of lines is processed to produce a summed line absorption coefficient for the wavelength interval of interest, including radiative, Stark, and van der Waals broadening. The line center opacity is also saved for each line for subsequent computation of the central depth.

In the second group of lines, each line has its individual source function, which is taken to be the Planck function if the calculation is LTE, and which is determined from the departure coefficients in the model in a non-LTE calculation. This group of lines is processed by directly computing the line opacity and source function at every wavelength point.

The spectrum is computed with a version of the model atmosphere program ATLAS [4] in which departure coefficients have been inserted in the partition

Atomic Data for Interpreting Stellar Spectra: Isotopic and Hyperfine Data

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Abstract

The quality of solar, stellar, and interstellar observations is now so high that we can see physical effects that have been assumed to be insignificant. In natural isotopic mixtures essentially all atomic lines are asymmetric because of isotopic and hyperfine components. In astrophysics the effects of isotopic components have been generally ignored in the case of Ti, Cr, Fe, and Ni. Ignoring isotopic splitting introduces the following systematic errors: 1) the use of bisectors to determine velocity fields is incorrect; 2) Fourier analysis of line profiles to determine rotational, microturbulent, and macroturbulent velocities is incorrect; and 3) damping constants are overestimated. When the stronger components become saturated, the weak components are still on the linear part of the curve of growth. This introduces the additional systematic errors: 4) wavelengths of saturated lines are shifted; and 5) abundances determined from equivalent widths are wrong. In addition the Doppler width and Voigt profile of each isotope are significantly different. It is imperative that laboratory measurements be made to determine the isotopic splitting of every energy level of every stable isotope of every atom and ion as is now routinely done for actinides and for diatomic molecules. Hyperfine splitting should be measured as well for those isotopes with nuclear spin. Russia, the United States, and other countries should stockpile pure stable isotopes so they will be available for these measurements. Computer programs for analyzing spectra including the hyperfine and isotopic splitting already exist. We now need the laboratory data.

1. Stellar Spectra

The spectrum of a star consists of many thousands of lines blended together. Even at infinite resolution and signal-to-noise the blends are difficult to interpret. At low resolution and signal-to-noise a spectrum does not contain enough information for interpretation. Without a priori information from other sources, the analysis of such a spectrum is usually incorrect. I believe that we can learn more by studying the brightest stars with the highest possible resolution and signal-to-noise, than from any number of lesser-quality observations of fainter stars.

ATOMIC DATA FOR INTERPRETING STELLAR SPECTRA: ISOTOPIC AND HYPERFINE DATA

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Presented at the 4th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas, September 14-17, 1992, Gaithersburg, Maryland.

To be published in *Physica Scripta*